How different can colours be? Maximum separation of points on a spherical octant

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The problem of determining n different colours that are as distinct as possible can be formulated as finding n points on a spherical octant that maximize the minimum distance between the points. We will determine the maximum separation distance and all extremal configurations for $n = 2$, 3, 4, 5 and 6. Conjectures are given for $7 \leqslant n \leqslant 15$.

Keywords: maximum separation problem; Tammes's problem; separation of colours

1. Introduction

It is well known that any colour can be decomposed into a non-negative linear combination of three basic colours, e.g. red, green and blue. The coefficients in this combination represent the contributions of each of the basis colours to the intensity and are therefore positive. Colours of a given intensity can be represented as points on a sphere that lie in the positive octant. Trying to find n different colours of equal intensity that are as distinct as possible is therefore equivalent to placing n points on a spherical octant such that the minimal distance between the points is as large as possible. For the sake of simplicity, it is assumed that colour resolution in the perception of the light detector (camera, human eye) is related to the Euclidean distance in this colour representation. The induced metric on the spherical octant is therefore that of Euclidean three-space or, equivalently, the metric on the surface of the sphere. A practical application is the recent and forthcoming work on the labelling of chromosomes (see Castleman 1993; van Kempen 1995; Nederlof 1991). We will concentrate here on the mathematical problem.

The type of maximum separation problems that is addressed here has been studied for several geometries. It is often equivalent to a circle packing problem. For a circular disc, results can be found in Coxeter *et al.* (1968), Melissen (1994*b*) and Pirl (1969), for a square in Kirchner and Wengerodt (1987), Melissen (1994*a*), Nurmela & Östergård (1998), Peikert *et al.* (1991), Schaer & Meir (1965), Schaer (1965), Schwartz (1970) and Wengerodt (1983, 1987*a*,*b*), and for an equilateral triangle, Melissen (1993, 1994*b*), Melissen & Schuur (1995) and Oler (1961). There is an enormous amount of literature dealing with the problem on a two-sphere in three-space

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where it is known as Tammes's problem (Tammes 1930), but exact solutions are known only in a few special cases. The best arrangements for 3, 4, 6 and 12 points have been found by L. Fejes Tóth (1943); Schütte & Van der Waerden (1951) and Van der Waerden (1952) described the optimal configurations for $n = 5$, 7, 8 and 9; Danzer (1963) did so for $n = 10$ and 11; Lee (1994) for $n = 13$ and 14; and Robinson (1961) for 24 points. Simpler proofs for $n = 10$ and 11 were given by Böröczky (1983) and Hárs (1986). Various upper and lower bounds have been constructed for other values of n (see Croft *et al.* 1991; Fejes Tóth 1972; Kottwitz 1991 and references therein). Optimal arrangements on a hemisphere can be found in Kertész (1994) and Melissen (1997), a ball is treated by Blachman (1963), Hadwiger (1952); for a cube see Goldberg (1971), Schaer (1966*a*–*c*, 1994) and for several polyhedra Bezdek (1987). Coxeter (1985), Lachs (1963) and Mackay (1980) considered the three-sphere in four-space.

In this article we address the maximum separation problem for a closed spherical octant in Euclidean three-space, a problem that is closely related to both the Tammes problem and the maximum separation problem in a square in the plane. The minimum distance between n points on the closed positive octant $\mathcal{O}$ of the unit sphere is called the *separation distance*. The maximum possible separation distance for n points on $\mathcal{O}$ will be denoted by o_n. We will determine o_n for $n \leqslant 6$ (for $n = 5$ and 6, the proofs are sketched) and conjectures are given for $7 \leqslant n \leqslant 15$.

2. Contraction on the octant

For some of the proofs that follow it is useful to know that, if there can only be finitely many configurations of n points that have a separation distance of at least d, then d must be equal to o_n. This clearly holds, for instance, for maximum separation configurations in a convex body in Euclidean space, because any homothetic image with a factor smaller than 1 can be moved slightly inside the body, showing that there are infinitely many configurations when the separation distance is smaller than the optimal value. To show that this is also true on the octant we must find a homotopy $\lambda \mapsto T_\lambda$ of maps T_λ that reduce all positive distances for $\lambda < 1$, and where T_1 is the identity map. As the existence of such a homotopy is not entirely obvious (it does not exist on the sphere, for instance), we devote some attention to it.

The map that is proposed reduces distances along the sphere to its north pole by a factor $\lambda \leqslant 1$. In spherical coordinates we have

$$T_\lambda(\boldsymbol{x}) = \begin{pmatrix} \cos\varphi \sin\lambda\theta \\ \sin\varphi \sin\lambda\theta \\ \cos\lambda\theta \end{pmatrix}, \quad \text{where } \boldsymbol{x} = \begin{pmatrix} \cos\varphi \sin\theta \\ \sin\varphi \sin\theta \\ \cos\theta \end{pmatrix}.$$

On the northern hemisphere this map satisfies our needs, because

$$|T_\lambda(\boldsymbol{x}_1) - T_\lambda(\boldsymbol{x}_2)|^2 = 2(1 - \cos(\varphi_1 - \varphi_2)\sin\lambda\theta_1 \sin\lambda\theta_2 - \cos\lambda\theta_1 \cos\lambda\theta_2),$$

so

$$\begin{aligned} |\boldsymbol{x}_1 - \boldsymbol{x}_2|^2 - |T_\lambda(\boldsymbol{x}_1) - T_\lambda(\boldsymbol{x}_2)|^2 &= 2[-\cos(\varphi_1 - \varphi_2)(\sin\theta_1 \sin\theta_2 - \sin\lambda\theta_1 \sin\lambda\theta_2) \\ &\qquad + \cos\lambda\theta_1 \cos\lambda\theta_2 - \cos\theta_1 \cos\theta_2)] \\ &\geqslant 2[\cos\lambda\theta_1 \cos\lambda\theta_2 + \sin\lambda\theta_1 \sin\lambda\theta_2 \\ &\qquad - \cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2] \end{aligned}$$

Table 1. *Maximum separation distance* o_n
(Conjectures for $n \geqslant 7$.)

n	o_n		
2	$\sqrt{2}$	$=$	$1.4142135623\ldots$
3	$\sqrt{2}$	$=$	$1.4142135623\ldots$
4	$\sqrt{2-2/\sqrt{3}}$	$=$	$0.9194016867\ldots$
5	equation (6.1)	$=$	$0.8194300004\ldots$
6	$\frac{1}{3}\sqrt{18-2\sqrt{29+4\sqrt{7}}}$	$=$	$0.7758146081\ldots$
7	$\sqrt{2-2\sqrt{(5+2\sqrt{5})/15}}$	$=$	$0.6408518201\ldots$
8			$0.5953339243\ldots$
9			$0.5579977161\ldots$
10			$0.5285245682\ldots$
11			$0.4852601255\ldots$
12			$0.4689998644\ldots$
13			$0.4416348424\ldots$
14			$0.4241017007\ldots$
15			$0.4125941130\ldots$

$$= 4\sin(\tfrac{1}{2}(1+\lambda)(\theta_1+\theta_2))\sin(\tfrac{1}{2}(1-\lambda)(\theta_1+\theta_2)) > 0,$$

as $\theta_1+\theta_2 \leqslant \pi$ and $\lambda < 1$.

3. Two points

The distance between two points on $\mathcal{O}$ is at most equal to $\sqrt{2}$,

$$\|\boldsymbol{x}-\boldsymbol{y}\|^2 = 2(1-\boldsymbol{x}\cdot\boldsymbol{y}) \leqslant 2.$$

The upper bound $o_2 = \sqrt{2}$ can only be assumed if one of the points is a vertex of $\mathcal{O}$. The other point must then lie somewhere on the opposite edge (see figure 1*a*).

4. Three points

If the three points are placed in the corners of $\mathcal{O}$, their mutual distances are equal to $\sqrt{2}$. By the previous argument, this value is maximal and the configuration in figure 1*b* is evidently unique.

5. Four points

At first, finding an optimal position for only four points may appear trivial. The solution that suggests itself has three points at the vertices of $\mathcal{O}$ and one at the centre. The separation distance is then equal to $o_4 = \sqrt{2-2/\sqrt{3}}$. However, there happens to be a second, equally good arrangement that has one point at a vertex, two points are at distance o_4 from this point on each of the adjacent edges and a

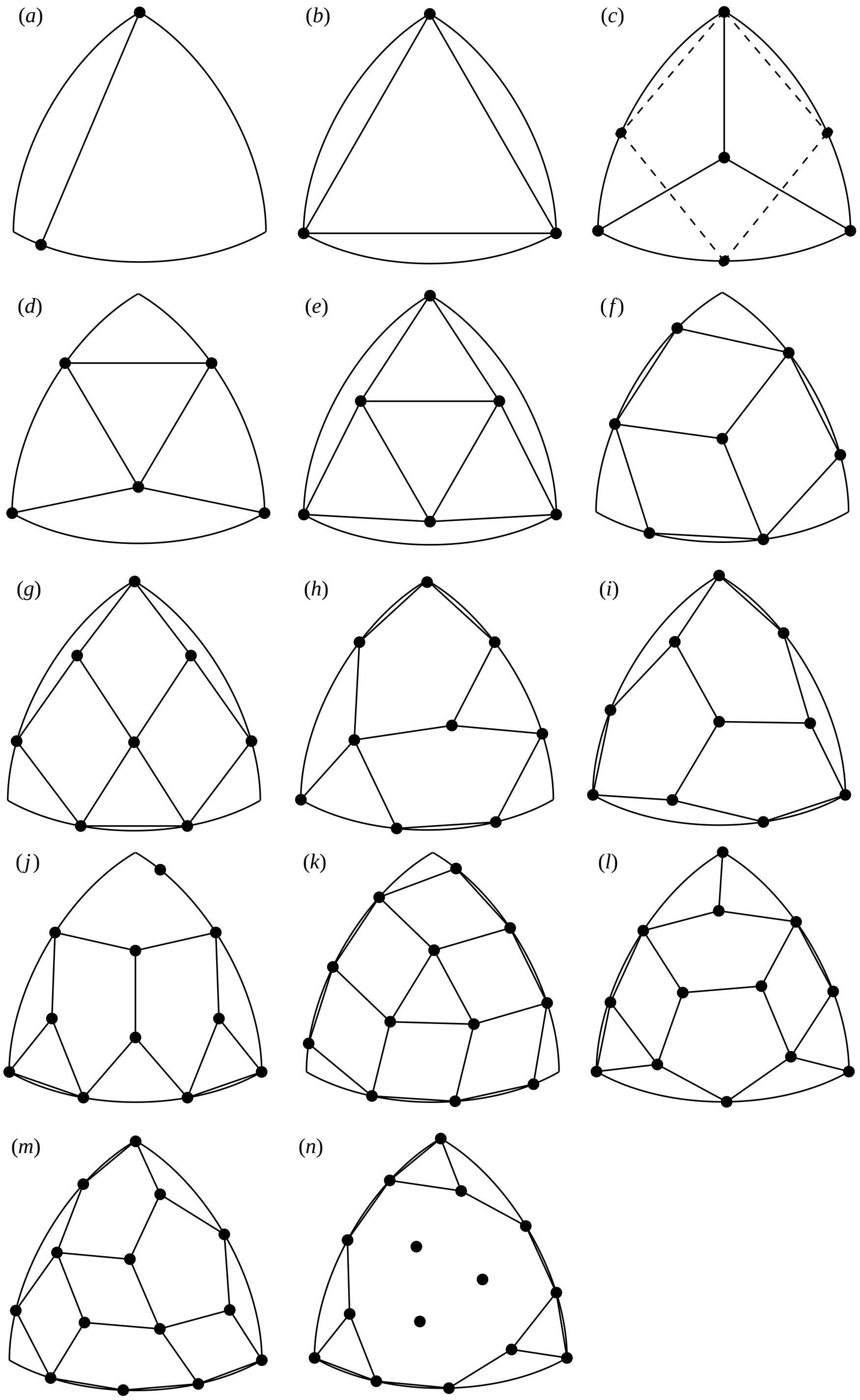

Figure 1. Optimal ($n \leqslant 6$) and conjectured maximum separation arrangements of n points on a spherical octant shown in a projection along $(1, 1, 1)$. The solid and dashed line segments are of length o_n (see table 1).

fourth point lies at the middle of the opposite edge (the dashed configuration in figure 1*c*). There are obviously three such configurations.

To prove that these are all the optimal configurations, suppose that the separation distance of four points in $\mathcal{O}$ is equal to o_4. We will show that this permits only configurations that are congruent with one of the arrangements in figure 1*c*.

The configuration can always be rearranged by rigid motions and by increasing distances to ensure that at least three points lie on the boundary $\partial\mathcal{O}$. First, suppose that all four points are on the boundary. One of the closed edges must then contain two points: p_1 and p_2. Their distance can be assumed to be equal to o_4, because otherwise they can be moved closer together along the boundary without decreasing the separation distance. Likewise, the two other points p_3 and p_4 can be assumed to have a distance o_4 to p_1 and p_2, respectively. The coordinates of these points can be parametrized as follows:

$$p_1 : (\cos\varphi, \sin\varphi, 0), \quad p_2 : (\cos(\varphi+\varphi_0), \sin(\varphi+\varphi_0), 0),$$
$$p_3 : (x_3, 0, \sqrt{1-x_3^2}), \quad p_4 : (0, y_4, \sqrt{1-y_4^2}),$$

where

$$\varphi_0 = 2\arcsin\tfrac{1}{2}o_4, \quad x_3 = \frac{1}{\sqrt{3}\cos\varphi}, \quad y_4 = \frac{1}{\sqrt{3}\sin(\varphi+\varphi_0)}, \quad \varphi \in [0, \tfrac{1}{2}\pi - \varphi_0].$$

The distance between p_3 and p_4 can only exceed o_4 when

$$\left(1 - \frac{1}{3\cos^2\varphi}\right)\left(1 - \frac{1}{3\sin^2(\varphi+\varphi_0)}\right) < \frac{1}{3}. \tag{5.1}$$

To show that this cannot happen, the left-hand side can be bounded from below by using its symmetry and the inequalities

$$\cos\varphi \geqslant 1 - \tfrac{1}{6}\varphi, \quad \sin(\varphi+\varphi_0) \geqslant \sqrt{\tfrac{2}{3}}(1 + \tfrac{1}{2}\varphi),$$

which are valid for $\varphi \in [0, \frac{1}{4}\pi - \frac{1}{2}\varphi_0]$. The lower bound that is obtained in this way, can be differentiated with respect to φ,

$$4\frac{120 - 156\varphi - 18\varphi^2 - 7\varphi^3}{(6-\varphi)^3(2+\varphi)^3} \geqslant \frac{293}{6750} > 0,$$

as $0 \leqslant \varphi \leqslant \frac{1}{3}$. This shows that the left-hand side in equation (5.1) is at least equal to $\frac{1}{3}$, and this value is only assumed for $\varphi = 0$ and $\varphi = \frac{1}{2}\pi - \varphi_0$, which means that one of the points must be a vertex. This results in the dashed solution in figure 1*c*.

Second, let three points p_1, p_2 and p_3 of the configuration lie on the boundary of the octant, while the fourth point p_4 lies in its interior. Now consider figure 2*a*. The points in this figure are defined by

$$|a_1a_4| = |a_2a_5| = |a_5a_8| = |a_6a_9| = |a_9a_{12}| = |a_{10}a_1| = o_4.$$

The points a_3, a_7 and a_{11} lie on the centres of the arcs a_1a_5, a_5a_9 and a_1a_9, respectively, and a_{13} is the centre of $\mathcal{O}$.

By symmetry, it may be assumed that p_4 lies in the spherical triangle $a_1a_3a_{13}$. If p_4 coincides with a_{13}, then there is only room for three points at the vertices of the octant, which is the drawn solution in figure 1*c*. Suppose that this is not the case. The points p_1, p_2 and p_3 must lie on $a_4a_5a_9a_{12}$. The points p_1 and p_3 restrict

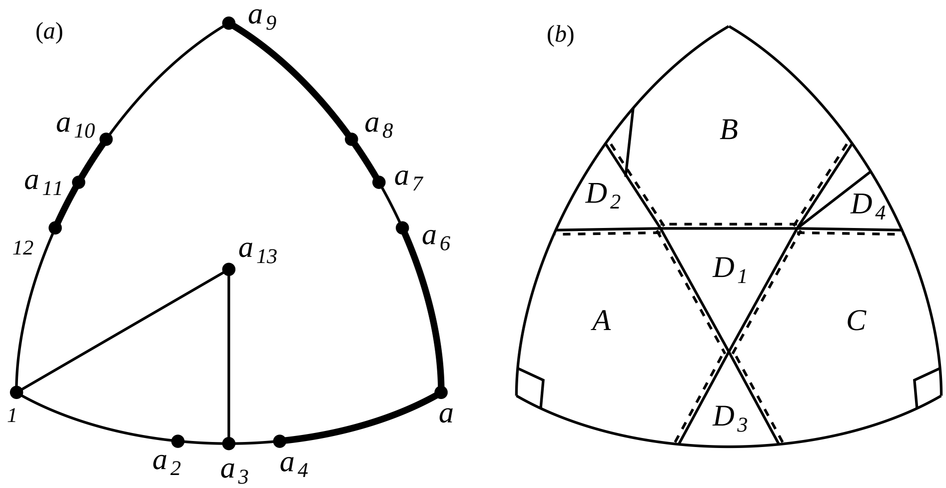

Figure 2. The points $a_1, \ldots, a_{13}$ and the partition for the proof of $n = 5$.

p_2 to lie between a_7 and a_9, so p_1 then lies on the arc between a_{10} and a_{12}, and p_3 is between a_4 and a_6. If p_1 is between a_{10} and a_{11}, then p_2 is between a_7 and a_8, and p_3 is between a_4 and a_5. The point p_4 can then be moved onto the arc between a_1 and a_2. From previous arguments we know that four points on the boundary are only possible if $(p_1, p_2, p_3, p_4) = (a_{10}, a_7, a_4, a_1)$ or if $(p_1, p_2, p_3, p_4) = (a_{11}, a_8, a_5, a_2)$. As these solutions are rigid, p_4 cannot lie in the interior. If p_1 is between a_{11} and a_{12}, then p_4 is in the triangle $a_2a_3a_{13}$, so p_3 is between a_5 and a_6, and p_2 is between a_8 and a_9. Now, p_4 can be moved onto the boundary between a_2 and a_3, and we are done again.

6. Five points

The best arrangement of five points is unique up to rotations and is shown in figure 1*d*. Its separation distance o_5 is the smallest positive root of

$$o_5^8 - 24o_5^6 + 112o_5^4 - 160o_5^2 + 64 = 0,$$

which is given explicitly by

$$o_5 = \sqrt{6 + \sqrt{h} - \sqrt{52 - h + 12\sqrt{h} - 2\sqrt{h^2 - 16h + 48}}} = 0.81943000041\ldots, \quad (6.1)$$

where

$$h = \tfrac{8}{3}\sqrt{7}\cos(\tfrac{1}{3}\arctan(\tfrac{3}{107}\sqrt{1167}) + 2\pi) + \tfrac{52}{3}.$$

We will give some geometrical arguments that prove the optimality and uniqueness of these configurations. The tedious but straightforward calculations that are needed to verify some geometrically obvious facts will be omitted.

Consider the partition shown in figure 2*b*. The vertices in this partition are equal to the positions of the points in figure 1*d* and its rotated copies. The three interior vertices are assigned to D_j ($j = 2, 3, 4$). None of the regions A, B and C can contain two points of the configuration, as there are only three different ways to accommodate two points in their closure. Likewise, the region $\mathrm{D} = \bigcup_{j=1}^{4} \mathrm{D}_j$ can contain at most

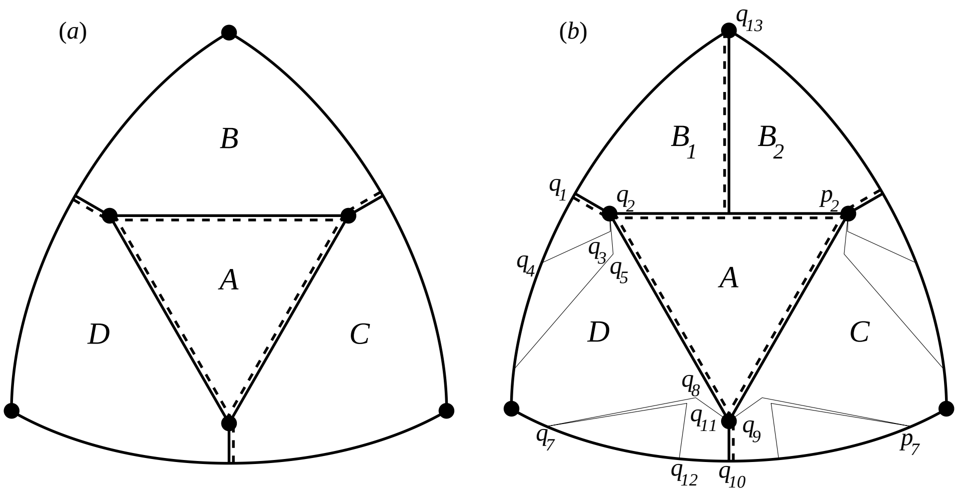

Figure 3. Partitions for the proof of $n = 6$.

three points. A point in D_1 prohibits other points from lying in D, so there can be no point in D. This leaves the following two possible situations.

(1) There is one point in each of A, B and C, as well as two points in $\bigcup_{j=2}^{4} D_j$, for instance, in D_3 and D_4. The points in D_3 and D_4 restrict the point in C to lie in a small region around the vertex of $\mathcal{O}$, as shown in figure 2*b*. This, in turn, restricts the points in D_4 and B. The same can be done for the point in A. It turns out that the points in A and B are too close together, their distance cannot exceed $0.62578\ldots < o_5$, so this situation cannot occur.

(2) There are two points in $A \cup B \cup C$ (for instance, in A and C), and one point in each of D_2, D_3 and D_4. The points in D_2, D_3 and D_4 restrict the points in A and B to a small region around the vertices of $\mathcal{O}$. The only possible position for the point in D_3 is the interior vertex. This fixes the positions of the points in A and B, and also of the points in D_1 and D_2, resulting in the solution in figure 1*d*.

7. Six points

We will demonstrate that the maximum separation distance of six points in $\mathcal{O}$ is given by

$$o_6 = \tfrac{1}{3}\sqrt{18 - 2\sqrt{29 + 4\sqrt{7}}} = 0.7758146081\ldots,$$

and that the unique optimal arrangement is the one in figure 1*e*. The points in the configuration in figure 1*e* are used to define the vertices in the partitions in figure 3.

Suppose that six points in $\mathcal{O}$ are at least o_6 apart. In region A there is room for at most one of these points, and B, C and D can each contain at most two points. The validity of this last statement is seen as follows. Divide region B into two subregions, B_1 and B_2, as in figure 3*b* and suppose that there are three points in B. If the vertex q_{13} is one of these points, there can be only one point in B_1 (q_2) and no point in B_2. If q_{13} is not part of the arrangement, there can be at most one point in B_1 and one in B_2.

First, let there be a point in A. Two other regions (for instance, C and D) must each contain two points. The regions C and D can each be subdivided into two subregions, just like B in figure 3*b*, so that each contains one point. Define the points q_j, and their mirror images p_j, for $1 \leqslant j \leqslant 12$ such that $o_6 = |q_1q_7| = |q_7q_8| = |q_8p_2| = |q_{11}p_7| = |q_1q_{11}| = |q_4q_{12}| = |q_3q_{12}| = |q_3p_2|$, and the obvious symmetrical relations.

The two points in D restrict each other to the regions $q_1q_2q_5q_6$ and $q_7q_8q_9q_{10}$, respectively. The last region is constrained by one of the points in C to region $q_7q_{11}q_{12}$. This restricts the other point in D to $q_1q_2q_3q_4$. The points in $p_1p_2p_3p_4$ and $q_1q_2q_3q_4$ restrict the point in A to a region with a z coordinate of at most $0.318279\ldots$, whereas the points in $p_7p_{11}p_{12}$ and $q_7q_{11}q_{12}$ require a z coordinate of at least $0.496737\ldots$, which is impossible.

As A cannot contain a point of the configuration, there must be two points in B, C and D. If one of these points happens to be a vertex of $\mathcal{O}$, the location of other points is unique, resulting in the configuration in figure 1*e*. The situation that no point is a vertex of $\mathcal{O}$ can be eliminated as before. All points can be restricted to lie in regions like $q_1q_2q_3q_4$. Two points in D and B_1 now have a distance of at most $0.497545\ldots < o_6$.

8. Seven to fifteen points

The (conjectured) best configurations with up to eight points exhibit forms of symmetry, but for nine points the best solution appears to be non-symmetric. For ten points, the best configuration encountered is again symmetric. The optimal distance is the smallest positive zero of

$$169d^8 + (584\sqrt{3} - 880)d^6 - (2560\sqrt{3} - 3376)d^4 - (9088 - 2688\sqrt{3})d^2 + 4864 - 2048\sqrt{3}.$$

The configuration that is shown in figure 1*k* for eleven points has the interesting feature that one of the points has some freedom of movement. The other points lie symmetrically in the octant. The arrangement for thirteen points is virtually symmetric. However, close inspection reveals that one of the points that appears to lie on the boundary of the octant in fact does not! With a separation distance of $0.4416348424\ldots$, this configuration is slightly better than the nearby symmetric one, which has a separation distance of $0.4411307339\ldots$. The configuration for fourteen points again lacks symmetry. For fifteen points there are three points that have some limited freedom of movement. The separation distance in this configuration is the smallest positive zero of

$$d^{20} - 16d^{18} + 116d^{16} - 528d^{14} + 1732d^{12} - 4320d^{10} \\ + 8512d^8 - 13440d^6 + 14848d^4 - 8192d^2 + 1024.$$

The conjectured arrangements have been obtained by a repeated numerical maximization of the separation distance of n points, starting from random initial arrangements. For the arrangements that suggest themselves the separation distance was calculated analytically or as the root of a polynomial (see table 1).

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